



**REACH: Exposure scenarios for preparations
Methodology for the identification of substances that represent
the dominant risks to human health and/or the environment and
the drivers for risk management measures**



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Disclaimer

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Important note to the reader – DPD+-Method

Status of the current document:

Although the DPD+ methodology is still under testing, Cefic decided to publish this document on their website to inform industry about the methodology that has been recognised by industry and ECHA as a valuable alternative to the methodology described in the ECHA Downstream User Guidance.

The principles underlying the DPD+-method will be maintained and will be more refined with the outcome of further review and testing exercises.

The methodology has been developed and tested based on a limited set of chemistries and applications. Further additional practical testing with different preparations and endpoints is required to explore and refine the applicability and usability of the method.

Scope of the DPD+-method:

The DPD+-method represents an element for implementing the REACH Guidance for Downstream Users when a preparation contains more than one dangerous substance. Assuming that the control of the lead substance(s) warrants appropriate control of all other preparation constituents, the complexity of multi-substance preparations can be reduced and the communication of Exposure Scenarios in the supply chain can be focused on the lead substance(s) Exposure Scenarios.

The DPD+ method is the first tier-element in the identification of the lead substance(s) in a preparation. It relies on of the long-established, and widely familiar procedures for classification of Dangerous Preparations for their health and/or environmental effects (see The Dangerous Preparations Directive, 1999/45/EU), enhanced for certain health exposure pathway with consideration of the volatility of the substance(s) concerned. Hence, it is referred to as the “DPD+ method”.

The identification of lead substances in preparations containing safety-relevant concentrations of substances which are classified as category 1 or 2 carcinogenic, mutagenic or reprotoxic, as respiratory sensitizers or which are identified PBT-, or vPvB-substances is beyond the scope of the DPD+-method. Preparations containing safety-relevant concentrations of such substances will require an advanced evaluation. For some other properties it still has to be checked whether they should trigger additional steps and/or expert judgement (e.g. corrosivity or the formation of non volatility depended aerosols). Complementary elements are under development (see above) to improve the lead substance identification

Outlook on ongoing developments:

This guidance document will continue to be enhanced as experience with this guidance is gained. Further additional practical testing with different preparations and endpoints is required to explore and refine the applicability and usability of the method. A project has been initiated by Cefic / VCI to test this DPD+ guidance for several examples.

The outcome of this project will be used to develop complementary elements needed for identifying the lead substances in preparations which fall out of the Scope of the DPD+-method. The DPD+-method together with complementary elements will provide a consistent rule set for an objective identification of the lead substances in preparations. Such a rule set is a prerequisite for selecting the relevant substance Exposure Scenarios to ensure the safe use of preparations.

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1. Introduction

1. The REACH Regulation introduces many new, and in some case, significantly different, requirements on all actors involved in the supply and use of a chemical (“substance”) from those set out in previous legislation relating to protection of human health and of the environment from the uses of substances.

2. A number of REACH requirements apply to companies who manufacture preparations (mixtures of substances, as such, and/or other preparations), who are required to pass on information on safe uses to the remainder of the use chain they supply into. In turn, their customers may be required to pass comparable information on to their user/customer base. REACH requires provision of more comprehensive and detailed information than previously supplied, with the introduction of an extended safety data sheet, with the addition of exposure scenarios (“ES”) for each use. An ES provides specific information on how a substance is to be managed and controlled under specified circumstances of use, to ensure the use is safe to man and/or to the environment.

3. The procedures set out in REACH regarding information flows down supply and use chains do not adequately address the practicalities associated with the handling and management of data relating to the many substances present in a typical preparation. As the approach identifies the lead substance of a preparation, its applicability is not restrained by the number of substances and the percentage of hazardous substances in the preparation.

4. Efficient communication of safe use data to downstream users of preparations depends on adoption of procedures that enable the formulator of a preparation to identify and to extract key and relevant information from the detailed information he receives on the materials used in the preparation (recognising that simply passing on all information received to the next actor in the use chain would be counter-productive to the aims of REACH).

5. Guidance and a methodology for identification of so-called “critical components” in a preparation, and the subsequent development of an exposure scenario, are included in the ECHA guidance for downstream users (download: http://guidance.echa.europa.eu/docs/guidance_document/du_en.pdf). Industry review of this approach has identified a number of weaknesses, which limit its value.

6. An alternative industry-developed methodology has been prepared (ESIG-FEICA), which was presented to peer-industry manufacturer and formulator sectors, the European Commission, ECHA and selected member states (Commission Varese Workshop, May 2008). The principles demonstrated at this meeting were widely supported, and a number of refinements and modifications were agreed from the meeting. Whilst there was official support for the approach, the authorities sought greater assurance on the applicability and usability of the methodology. The authors were encouraged to prepare a draft methodology for evaluation by downstream manufacturers of preparations, whether for intended use as components of other preparations, or in their finished state. The methodology outlined here, represents one way of implementing the preparation workflow of page 115 of the DU guidance. It is not a replacement to this workflow (See Appendix 2). [Note: this document is based on the Dangerous Preparations Directive (DPD) classification scheme, with which industry is very familiar. The principles underlying the methodology can equally be applied to the GHS-classification scheme, which will replace the DPD classification scheme, and will be included in later versions of this document.]

7. This document sets out the methodology, which is freely circulated and provided for practical evaluation by any preparation manufacturer.

2. Description and principles

8. The method is based on use of the long-established, and widely familiar procedures for classification of Dangerous Preparations for their health and/or environmental effects (see The Dangerous Preparations Directive, 1999/45/EU), enhanced for certain health exposure pathway with consideration of the volatility of the substance(s) concerned. The proposed approach is referred to as the “DPD+ method”. The method is the first tier-element of a tiered approach to the selection of the relevant substance Exposure Scenarios that will be used to provide the risk management measures and operational conditions to ensure the application of a preparation is safe. It has to be supplemented by an additional assessment step if e.g. preparations contain substances which are classified as category 1 or 2 carcinogenic, mutagenic or reprotoxic or as respiratory sensitizers. It is also not applicable to PBT-, or vPvB-substances. Preparations containing relevant concentrations of such substances will require an advanced evaluation. Such substances should be dealt with individually and the OCs/RMMs applicable to the individual substance complied with.

9. As with the Dangerous Preparations Directive, account is taken of individual health exposure pathways and end points for the aquatic environment. The outcome of application of the DPD+ method to a preparation is the identification of the so-called “lead substance” for each relevant health exposure pathway and for the aquatic environment. For any given exposure pathway or emission route, the substance with the highest classification impact is considered to be the lead substance for that effect.

10. To facilitate comparisons, in general the concentration limit (C_L) where a dilution has no longer to be classified is taken into account.

Example: a substance labeled with R24 (toxic in contact with skin) at a concentration $\geq 25\%$ has a boundary concentration of 3% for labelling with R21 (harmful in contact with skin). Therefore, in this case 3% is the concentration limit C_L .

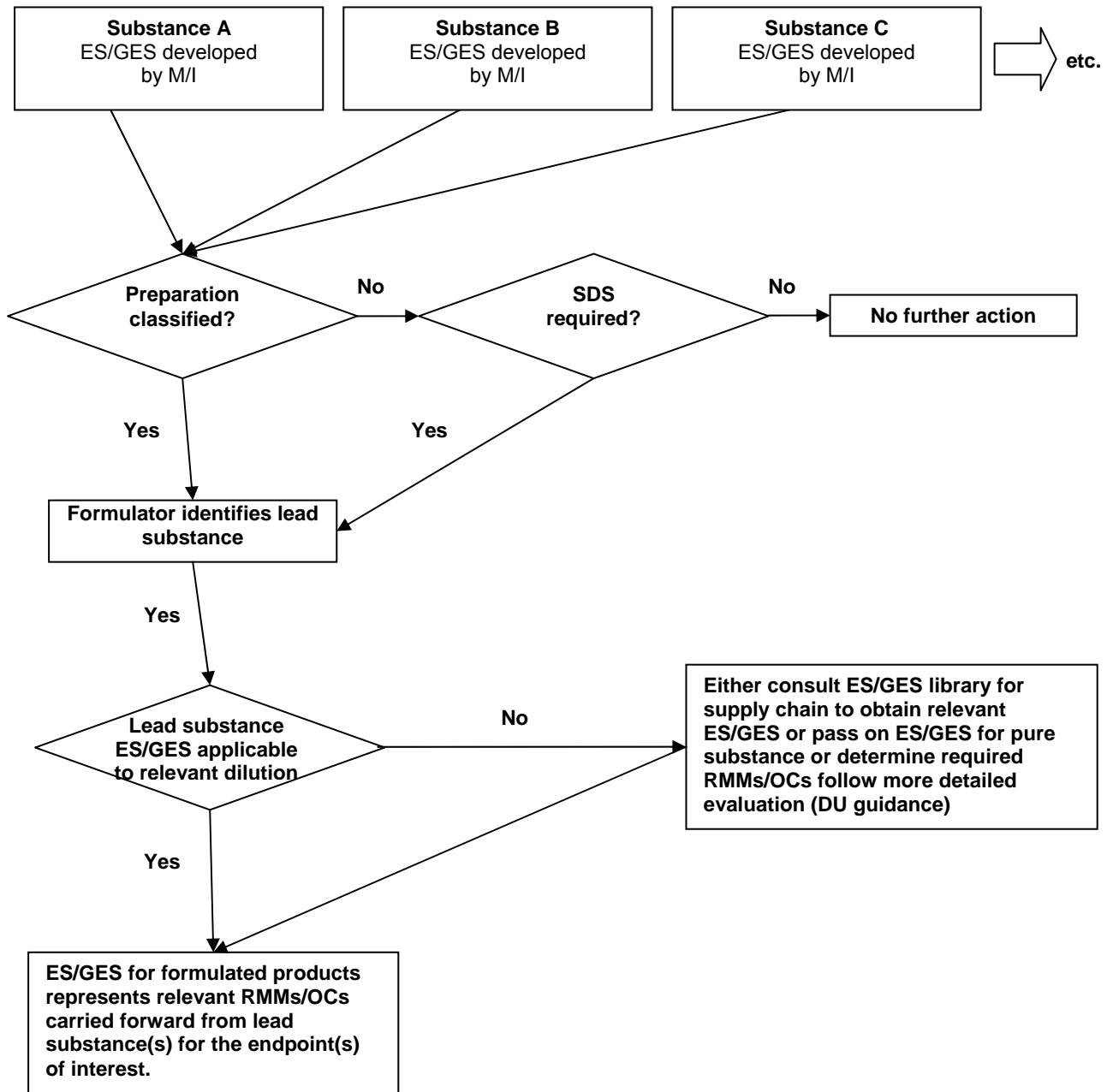
11. The impact of a substance on the classification of a preparation is determined as the ratio of the substance concentration (C_i) to the concentration limit (C_L). This ratio C_i/C_L is calculated for each dangerous substance and each exposure pathway/emission route. It is termed the “lead substance indicator (LSI)”. The substance with the highest LSI is deemed to have the highest impact and thus is the lead substance for a given exposure or emission pathway. [Note: identification of a particular lead substance does not necessarily result in the preparation being classified for that particular effect].

12. More than one substance, classified for the same human health end point, which is recognised to be additive, may be present in the preparation. In such cases, the total amount of the substances concerned is taken into account and the overall composition of the whole preparation may need to be considered in identifying appropriate risk management measures.

13. Once the lead substance(s) have been identified, the information provided in the respective substance ES for the relevant use(s), related to the exposure pathway and/or emission route concerned, is used to prepare the ES for the preparation.

Figure 1 provides an overview of the process.

14. Figure 1: overview of methodology



3. Methodology

Step 1: substance profile of the preparation

15. This step requires the overall formulation of the preparation to be expressed in terms of its constituent substances. It is necessary to break down any raw materials and intermediates, which themselves are preparations.

Where the exact composition of a raw material is not known, the upper end of any concentration range given in the safety data sheet or technical data sheet should be used. The volatility should be indicated by recording the vapour pressure of the preparation ingredients (see Chapter 9 of the respective safety data sheets). A default value of 10^{-6} hPa is chosen for inorganic and polymeric substances.

Table 1: example preparation breakdown

A	B	C	D	E	F	G
Preparation		Breakdown		Overall Composition		Vapour pressure (hPa at 25°C)
Component	%	Component	%	Component	%	
Titanium dioxide	25.00	Titanium dioxide	25.00	Titanium dioxide	25.00	< 10^{-6}
Resin solution A	30.00	Epoxy polymer	18.00	Epoxy polymer	18.00	< 10^{-6}
		Xylene	12.00) Xylene	27.00	7-9
Xylene	15.00					
Resin solution B	15.00	Melamine-formaldehyde polymer	10.50	Melamine-formaldehyde polymer	10.50	< 10^{-6}
		Toluene	4.50) Toluene	4.75	29
Silicon flow agent	0.50	Toluene	0.25			
		Polysiloxane	0.25	Polysiloxane	0.25	< 10^{-6}
Ethyl acetate	14.5			Ethyl acetate	14.50	103

Step 2: substance classification

16. For each substance identified in Step 1, identify and fill in columns H, J, K or L of Table 2:

- the substance name
- the hazard classification, as expressed by R-phrases (*either* from Annex I of the Dangerous Substances Directive *or*, in the case of substances not officially classified, but self-classified, from the supplier's safety data sheet)
- the concentration limit applicable to each R-phrase identified (*either* the default limit(s) from Annexes II, III and V of the Dangerous Preparations Directive *or*, from the Annex I entry, if the substance is assigned a specific concentration limit, which applies over the default limit)

[Notes: Appendix 1 lists the R-phrases and related exposure pathways and emission routes.]

Table 2: substance R-phrases and specific concentration limits

<i>H</i>	<i>J</i>			<i>K</i>	<i>L</i>
Substance (from Column E)	R-phrase(s)			Default concentration limit (%)	Specific concentration limit (%)
	Inhalation	dermal	environment		

4. Determination of the lead substance(s)

17. From information in Tables 1 and 2 complete Table 3.

18. In Column(s) 6, 9, 12, identify the substance(s) with the highest LSI value.

[Note: where the LSIs of two substances are equivalent or differ by a factor of less than 10%, each substance should be identified.]

5. Generation of the ES for the preparation

19. Carry out the following steps:

19.1 Determine which SU(s), PROC(s), PC(s), AC(s) and ERC(s) are relevant to the uses/applications of the preparation under consideration. Verify that for each constituent ESs are available for the relevant SU(s), PROC(s), PC(s), AC(s) and ERC(s) covering the constituents' dilution in the product and appropriate risk management measure (see Chapters 5 and 6 of the DU guidance for further detail).

19.2 Complete Section 1 of the standard ES format with the information from the step above

19.3 Complete Sections 2, 4.1 and 4.2 of the standard ES format with information relating to the composition and intended uses of the preparation, as included in product technical data sheets and/or the product safety data sheet.

19.4 For the lead substances identified above, obtain the ES(s) relevant to the uses/applications identified above.

[Note: before the final date for Registration of substances, only a proportion of the required ESs will be available. At any one point in time, downstream users are required in REACH only to use the information that is available, or made available to them, at that time. It is not expected or required that downstream users seek or provide data not yet provided by manufacturers or importers in Registration dossiers.]

19.5 From the ES for the relevant substance, extract the Operating Conditions (OCs) and Risk Management Measures (RMMs) applicable to the exposure and/or emission route in question.

19.6 Enter all the information on Operating Conditions (OCs) and Risk Management Measures (RMMs) applicable to the exposure and/or emission route in question into Sections 3, 4.3, 5, 6, and 7 of the standard ES format.

19.7 Review all information in Sections 3, 4.3, 5, 6 and 7 and edit to remove any replication and ensure there are no inconsistencies in the information from the individual substance ESs. In the event that there are differences, the highest or most demanding OC and/or RMM must be selected.

19.8 Complete Sections 8 and 9 of the standard ES format.

Table 3.1: determination of lead substance(s) - Example: Contact adhesive

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
Substance (Col H)	Conc'n in prep (Col F) (%)	Vapour press (Col G) (hPa)	Inhalation			Dermal			Eyes			Ingestion			Aquatic		
			R phrase (s) (Col J)	Conc'n limit (Col K or M) (%)	LSI [Col 3 x Col 2/Col 5]	R phrase (s) (Col J)	Conc'n limit (Col K or M) (%)	LSI [Col 2/ Col 8]	R phrase (s) (Col J)	Conc'n limit (Col K or M) (%)	LSI [Col 2/ Col 11]	R phrase (s) (Col J)	Conc'n limit (Col K or M) (%)	LSI [Col 2/ Col 14]	R phrase (s) (Col J)	Conc'n limit (Col K or M) (%)	LSI [Col 2/Col 14; if R50:Col 2/ (3 X Col 17)]
Ethyl Acetate	30.0	103	R67	25	124	R66	20	1.5	R36	20	1.5						
Cyclo-hexane	30.0	104	R67	25	125	R38	20	1.5			1.5	R65			R50/53	0.25	120
n-Hexane (Annex 1)	2.5	160	R48/20 R62 R67	5 5 25	80 80 16	R38 R48/20 R62	20 20 5	0.125 0.125 0.5				R65			R51/53	2.5	1
Naphtha hydrotreated light	20.0	120	R67	25	96	R66	20	1				R65			R51/53	2.5	8
Rosin	0.5	< 10 ⁻⁶	-	-	-	R43	-								-	-	-
Polychlorobutiene	17	< 10 ⁻⁶	-	-	-	-	-								-	-	-

The following lead substances have to be taken into account for the safety assessment:

- Inhalation: cyclohexane, ethyl acetate, naphtha hydrotreated (light), and n-hexane. Reasoning: 82,5% of the ingredients are classified R67 (drowsiness) leading to an overall LSI of 361.
- Dermal: n-hexane & cyclohexane. Reasoning: the critical effect skin irritation (R38) refers to both substances. Note: The specific concentration limits of n-hexane (Annex 1) takes precedence over the default values in the appendix.
- Eye: ethyl acetate (critical effect: eye irritation, R36)
- Oral: no lead substance. Classification R65 (may cause lung damage if swallowed) will only become relevant, if for the preparation in addition also the viscosity criterion laid down in Annex VI chapter 3.2.3 is fulfilled.
- Environment: Cyclohexane. Reasoning: LSI of 120 >> next highest LSI. No additive effects expected.

Table 3.2: determination of lead substance(s) - Example: Surface Treatment Product – The DPD+-method is not applicable.

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
Substance (Col H)	Conc'n in prep (Col F) % <i>(by weight)</i>	Vapour press (Ps) (Col G)	Inhalation			Dermal			Eyes			Ingestion			Aquatic		
			R phrase (s) (Col J)	Conc'n limit (Col K or M)	LSI <i>[Col 3 x Col 2/Col 5]</i>	R phrase (s) (Col J)	Conc'n limit (Col K or M)	LSI <i>[Col 2/ Col 8]</i>	R phrase (s) (Col J)	Conc'n limit (Col K or M)	LSI <i>[Col 2/ Col 11]</i>	R phrase (s) (Col J)	Conc'n limit (Col K or M)	LSI <i>[Col 2/ Col 14]</i>	R phrase (s) (Col J)	Conc'n limit (Col K or M)	LSI <i>[Col 2/Col 14; If R50:Col 2/ (3 X Col 17)]</i>
Water	58	23400 Pa	-			-			-			-			-		
Phosphoric acid	6	< 0.0001 Pa	R34	5	1,2	R34	5	1,2	R34	5	1,2	R34	5	1,2	-		
Manganese bis (dihydrogen- phosphate	8	< 0.0001 Pa	-						-			-			-		
Methylmorpholine N-oxide	3,5	0.25 Pa	-						-			-			-		
Nickel salts	2,5	< 0.0001 Pa	R42 R40	1 1	0,00025 0,00025	R43 R40	1 1	2,5 2,5	-			R22			R50/53	2,5	1
Ammonium phosphate	4,5	< 0.0001 Pa	-						-			-			-		
Zinc dihydrogen- phosphate	17,5	< 0.0001 Pa	-						-			R22			R50/53	2,5	7

Conclusion: The preparation ingredient 'nickel salts' is a respiratory sensitizer and classified R42. For that reason, the preparation requires a more in-depth evaluation with regard to the annex of the SDS.

APPENDIX 1

Relationship between classification, default concentration limit (for classification according to the Dangerous Preparations Directive) and the exposure pathway or emission route

<i>M</i>	<i>N</i>	<i>P</i>
R-Phrase	Default concentration limit (Annex II, Annex III and Annex V of DPD)	Relevant exposure pathway or emission route
R20	25%	Inhalation
R23	3%	
R26	0.1%	
R34	5%	
R35	1%	
R37	20%	
R39 in combination with R23	1%	
R39 in combination with R26	0.1%	
R40	1%	
R42 ¹	1%	
R46 ¹	0.1%	
R48 in combination with R20	10%	
R48 in combination with R23	1%	
R49 ¹	0.1%	
R60 ¹	0.5%	
R61 ¹	0.5%	
R62	5%	
R63	5%	
R64	1%	
R67	25% ⁴	
R68 in combination with R20	10%	
R68 in combination with CMR 3	1%	
R21	25%	Dermal
R24	3%	
R27	0.1%	
R34	5%	
R35	1%	
R38	20%	
R39 in combination with R24	1%	
R39 in combination with R27	0.1%	
R40	1%	
R43	1%	
R45 ¹	0.1%	
R46 ¹	0.1%	
R48 in combination with R21	10%	
R48 in combination with R24	1%	
R60 ¹	0.5%	
R61 ¹	0.5%	
R62	5%	
R63	5%	
R64	1%	
R66 ^b	20%	
R68 in combination with R22	10%	

<i>M</i>	<i>N</i>	<i>P</i>
R-Phrase	Default concentration limit (Annex II, Annex III and Annex V of DPD)	Relevant exposure pathway or emission route
R68 in combination with CMR 3	1%	
R22	25%	Ingestion
R25	3%	
R28	0.1%	
R34	5%	
R35	1%	
R39 in combination with R25	1%	
R39 in combination with R28	0.1%	
R40	1%	
R45 ¹	0.1%	
R46 ¹	0.1%	
R48 in combination with R22	10%	
R48 in combination with R25	1%	
R60 ¹	0.5%	
R61 ¹	0.5%	
R62	5%	
R63	5%	
R64	1%	
R65 (analogy to R22)	25% ⁴	
R68 in combination with R22	10%	
R68 in combination with CMR 3	1%	
R34	5%	Eyes
R35	1%	
R36	20%	
R41	5%	
R53	25%	Aquatic environment
R52/53	25%	
R51/53	2.5%	
R50/53	0.25% ²	
R50	0.25% ^{2,3}	
	<p>1: Classification indicates the need for expert evaluation.</p> <p>2: Specific concentration limits for substances classified as R50 or R50/53 have been introduced. They need to be taken into account in the identification of the lead substance.</p> <p>3: R50 substances undergo rapid degradation and do not bioaccumulate. Hence, their risk the environment is lower than that of substances labeled R50/53. According to Chapter R16 of the ECHA Guidance on Information Requirements and Chemical Safety Assessment rapidly degrading substances wastewater treatment plant of 67% whilst R50/53 labeled substances may not be affected (no degradation). This corresponding difference in the risk indicator can be accounted for by a correction factor of 3 in order to reflect the increased removal efficiency of a municipal wastewater treatment plant for rapidly degrading substances. Please note that this factor is not used for actual risk assessment but for discriminating between substances according to their risk. The LSI algorithm for substance labeled R50 is then $C/C_L \times 3$.</p> <p>4: In analogy to R20 and R22, respectively.</p> <p>5: In analogy with R38.</p>	

APPENDIX 2

Correspondence between the workflow for handling ESs in preparations in the DU guidance (Fig. 14.2) and its adaptation in the DPD+method

Workflow element in Figure 14.2 of DU Guidance	Correspondence to the DPD+-method.
Step a	Covered in Step 1, item 15
Step b	Covered in Step 2, item 16
Step c	Outside the scope of the DPD+ guidance
Step d	Outside the scope of the DPD+ guidance
Step e	Outside the scope of the DPD+ guidance
Step f	Covered in Step 4, item 19.1.
Step g	Outside the scope of the DPD+ guidance
Step h	Covered in Step 4, item 19.1.
Step i	Covered in Step 4, item 19.1.
Step j	Covered in Step 4, item 19.1.
Workflows Chapters 5 and 6	Covered in Step 4, item 19.1.
Step k, l	Covered in Step 4, item 19.5 and 19.6.
Step l	Outside the scope of the DPD+ guidance
Step m	Covered in Step 3, item 17, 18.
Step n	Covered in Step 4, item 19.5.
Step o	Covered in Step 4, item 19.6.
Step p	Outside the scope of the DPD+ guidance
Step q	Outside the scope of the DPD+ guidance
Step r	Outside the scope of the DPD+ guidance